Green's Function Approach to the Bose-Hubbard Model

Matthias Ohliger[1] and Axel Pelster[2,3]

[1]*Institut für Physik und Astronomie, Universität Potsdam,*
Karl-Liebknecht-Straße 24/25, 14476 Potsdam, Germany
[2]*Fachbereich Physik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany*
[3]*Institut für Theoretische Physik, Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*
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We use a diagrammatic hopping expansion to calculate finite-temperature Green functions of the Bose-Hubbard model which describes bosons in an optical lattice. This technique allows for a summation of subsets of diagrams, so the divergence of the Green function leads to non-perturbative results for the boundary between the superfluid and the Mott phase for finite temperatures. Whereas the first-order calculation reproduces the seminal mean-field result, the second order goes beyond and shifts the phase boundary in the immediate vicinity of the critical parameters determined by the latest high-precision Monte-Carlo simulations of the Bose-Hubbard model. In addition, our Green's function approach allows for calculating the excitation spectrum at finite temperature and for determining the effective masses of particles and holes.

Introduction: Ultracold bosonic gases trapped in the periodic potential of optical lattices represent tunable model systems for studying the physics of quantum phase transitions [1, 2, 3, 4]. They are described by the Bose-Hubbard Hamiltonian which decomposes into two parts: $\hat{H} = \hat{H}_0 + \hat{H}_1$. The first term $\hat{H}_0 = \sum_i [U\hat{n}_i(\hat{n}_i - 1)/2 - \mu\hat{n}_i]$, with the on-site energy U and the chemical potential μ, describes the repulsion of more than one boson residing on a lattice site. It is local and diagonalizable in the occupation number basis for any lattice site. The second term $\hat{H}_1 = -J_{i,j} \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j$ with the hopping matrix element $J_{i,j} = J$ if the lattice sites i and j are nearest neighbors and $J = 0$ otherwise describes the hopping between two sites due to the quantum-mechanical tunneling effect. The competition between the two energy scales U and J determines the existence of two different phases. When the on-site energy is small compared to the hopping amplitude, the ground state is superfluid (SF) as the bosons are delocalized in a phase coherent way over the whole lattice. In the opposite case, where the on-site interaction dominates over the hopping term, the ground state is a Mott insulator (MI) where each boson is trapped in one of the respective potential minima.

This characteristic quantum phase transition of the Bose-Hubbard model has been studied extensively both with analytical [5, 6, 7, 8, 9] and numerical [10, 11, 12] methods for zero temperature, while less literature exists on the finite-temperature properties of this transition [13, 14, 15]. In this letter we work out a Green's function approach in order to determine the MI-SF phase boundary and the excitation spectrum in the Mott phase beyond the mean-field level for finite temperature with a hopping expansion. Our analytical findings compare well with the latest high-precision Quantum Monte Carlo simulations and allow to propose a thermometer for bosons in optical lattices. In the following we restrict ourselves to a spatially homogeneous system and neglect the effects arising from the additional harmonic confining potential, which is present in all experimental settings, like the for-

mation of a shell structure [16]. However, these effects could be taken into account by applying the local density approximation where the external potential is taken into account in form of a spatially dependent chemical potential.

Green's Function Approach: As all single-particle properties of a quantum many-body system are contained in its Green function, we base our calculation on this quantity. Because we are interested in describing a system at non-zero temperature, we use the imaginary-time formalism [17, 18]. Therein, the single-particle Green function is defined as the thermal average of the time-ordered product of a creation and an annihilation operator in Heisenberg representation

$$G_1(\tau', j'|\tau, j) = \text{Tr}\left\{\frac{e^{-\beta\hat{H}}}{\mathcal{Z}}\hat{T}\left[\hat{a}_{j,\text{H}}(\tau)\hat{a}_{j',\text{H}}^\dagger(\tau')\right]\right\}, \quad (1)$$

with $\hbar = 1$, $\beta = 1/k_B T$, and the partition function $\mathcal{Z} = \text{Tr}\{e^{-\beta\hat{H}}\}$. Because it is not possible to obtain analytic expressions for the eigenstates and eigenenergies of the full Bose-Hubbard Hamiltonian, we cannot calculate the Green function exactly. Instead, we aim at a perturbative treatment and calculate this quantity as a power series in the hopping matrix element $J_{i,j}$. As that parameter is small for the Mott phase, where the lattices are deep and the interaction between particles is strong, we refer to this treatment as a strong-coupling expansion. In order to employ this perturbative expansion for finite temperature, we make use of the Dirac interaction picture and write the imaginary-time evolution operator in form of a Dyson series,

$$\hat{U}(\tau, \tau_0) = \hat{T}\exp\left[-\int_{\tau_0}^{\tau} d\tau_1 \hat{H}_1(\tau_1)\right], \quad (2)$$

where the time dependence of the Dirac-picture operators is determined by the local Hamiltonian $\hat{H}_0$. With its help we can write the Green function as

$$G_1(\tau', i'|\tau, i) = \text{Tr}\left\{\frac{e^{-\beta\hat{H}_0}}{\mathcal{Z}}\hat{T}\left[\hat{a}_{i'}^\dagger(\tau')\hat{a}_i(\tau)\hat{U}(\beta, 0)\right]\right\}, \quad (3)$$

where the time-ordering operator acts also on the time variables which are resulting from the expansion of the Dirac imaginary-time evolution operator in (2). When we now expand perturbatively in powers of the tunneling matrix element J, the $(n-1)$th order contribution $G_1^{(n-1)}$ in (3) turns out to depend on the n-particle Green function of the *unperturbed* system as $G_n^{(0)}(\tau_1', i_1'; \ldots; \tau_n', i_n'|\tau_1, i_1; \ldots; \tau_n, i_n) = \left\langle \hat{T} \left[\hat{a}_{i_1'}^\dagger(\tau_1') \hat{a}_{i_1}(\tau_1) \ldots \hat{a}_{i_n'}^\dagger(\tau_n') \hat{a}_{i_n}(\tau_n) \right] \right\rangle^{(0)}$. In order to determine $G_n^{(0)}$ we cannot use standard Wick's theorem because the unperturbed Hamiltonian $\hat{H}_0$ is not quadratic in the Bose operators. Although the lack of Wick's theorem in the present situation prevents us from using the powerful perturbative technique based on standard Feynman diagrams, we can nevertheless simplify $G_n^{(0)}$ by decomposing it into cumulants. To this end, we follow an approach reviewed by Metzner [19] in the context of the fermionic Hubbard model which describes electrons in a conductor. This decomposition is based on the important observation that the on-site Hamiltonian $\hat{H}_0$ is local. Consequently, the unperturbed Green functions $G_n^{(0)}$ are also local and can be decomposed into time-dependent cumulants $C_n^{(0)}$. For instance, we have $G_1^{(0)}(\tau', i'|\tau, i) = \delta_{i,i'} C_1^{(0)}(\tau'|\tau)$ with the cumulant

$$C_1^{(0)}(\tau'|\tau) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} \left[\Theta(\tau - \tau')(n+1) e^{(E_n - E_{n+1})(\tau - \tau')} \right.$$
$$\left. + \Theta(\tau' - \tau) n\, e^{(E_n - E_{n-1})(\tau' - \tau)} \right] e^{-\beta E_n}, \qquad (4)$$

where $\mathcal{Z}^{(0)} = \sum_n e^{-\beta E_n}$ is the unperturbed partition function for a single-site system with the on-site energy eigenvalues $E_n = Un(n-1)/2 - \mu n$. With this decomposition, we can represent $G_1^{(n)}$ diagrammatically: We denote an n-particle cumulant at a lattice site by a vertex with n entering and n leaving lines with imaginary-time variables, so we have, for instance, for the first two cumulants

$$\xrightarrow[\tau'\quad\ \tau]{\ i\ } \quad = \quad C_1^{(0)}(\tau'|\tau), \qquad (5)$$

$$\underset{\tau_1'\qquad\ \tau_1}{\overset{\tau_2'\qquad\ \tau_2}{\times}}\,i \quad = \quad C_2^{(0)}(\tau_1', \tau_2'|\tau_1, \tau_2). \qquad (6)$$

Furthermore, the hopping matrix element is symbolized by a line connecting two vertices:

$$i \xrightarrow{\qquad} j \ = \ J_{ij}. \qquad (7)$$

With all this, we can set up the diagrammatic rules for calculating the nth order contribution of the Green function in J. First: Draw all possible combinations of vertices with total n internal as well as one entering and one leaving line. Second: Connect them in all possibles ways and assign time variables and hopping matrix elements to the lines. Third: Sum all site indices over all internal lattice sites and integrate all internal time variables from 0 to β.

We also note here that we have to sum all site indices over the *whole* lattice, no matter whether two sites in a diagram coincide or not. We make use of the translational invariance in imaginary time and transform all expressions to Matsubara space. In the *second* diagrammatic rule the integrals over the time variables have then to be replaced by sums over all bosonic Matsubara frequencies $\omega_m = 2\pi m/\beta$ with integer m where the sum of the incoming frequencies must equal the sum of the outgoing ones.

The formalism developed so far allows for calculating the Green function to any given order in the tunneling matrix element J. But because one of our main goals is to describe the phase transition between the Mott insulator and the superfluid phase, and it is well known in the theory of critical phenomena that such a transition is characterized by diverging long-range correlations [18, 20], we must employ a non-perturbative method which is achieved by summing an infinite subset of diagrams. In order to perform this task, we introduce the sum of all one-particle irreducible diagrams including their respective symmetry factors and multiplicities as

$$\mathcal{C}_1(\omega_m, \mathbf{k}) = \ \xrightarrow{\bullet} \ + \ \xrightarrow{\ \text{\Large$\bigcirc$}\ } \ + \ldots. \qquad (8)$$

The self-energy which describes the movement of a single particle in a many-body environment is defined as $\Sigma = 1/G_1^{(0)} - 1/G_1$ [17]. For our case, it can be written in the form $\Sigma(\omega_m, \mathbf{k}) = 1/G_1^{(0)}(\omega_m) - 1/\mathcal{C}_1(\omega_m, \mathbf{k}) + J(\mathbf{k})$, where $J(\mathbf{k}) = 2J \sum_{\nu=1}^{D} \cos(k_\nu a)$ is the D-dimensional lattice dispersion. For instance, the first order in the self-energy, which corresponds to a summation of all simple chain diagrams, yields $\tilde{G}_1(\omega_m, \mathbf{k}) = \left[1/G_1^{(0)}(\omega_m) - J(\mathbf{k}) \right]^{-1}$ with $G_1^{(0)}(\omega_m) = \sum_n \left[(n+1)/(E_{n+1} - E_n + i\omega_m) - n/(E_n - E_{n-1} + i\omega_m) \right] e^{-\beta E_n}/\mathcal{Z}^{(0)}$. We note that performing the limit $\tau' \searrow \tau$ in the Green function allows to obtain the quasi-momentum distribution needed to explain experimental time-of-flight absorption pictures [21, 22, 23].

Phase Boundary: The boundary of the phase transition is characterized by diverging long-range correlations [18, 20]. Thus, we set $\mathbf{k} = 0$ and solve for the value of J, where the Green function diverges, which is only possible for $\omega_m = 0$. This yields up to first order in J

$$2DJ_c = \frac{\sum_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n} \left(\frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}} \right)}, \qquad (9)$$

which coincides with the finite-temperature mean-field result [14, 15, 24]. The zero-temperature limit of (9), i.e. $2DJ_c = 1/\left(\frac{n+1}{E_{n+1} - E_n} - \frac{n}{E_n - E_{n-1}} \right)$, agrees with the seminal mean-field result of Ref. [1]. The reason for this agreement is that each approximation becomes exact in the limit of infinite spatial dimension. In order to
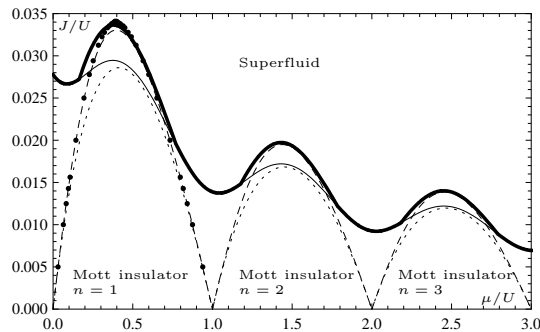
FIG. 1: Quantum phase diagram for $D = 3$. Thick (solid): Second (first) order, $k_B T = 0.1 \, U$. Dashed (dotted): Second (first) order, $T = 0$. Dots: QMC Data for $T = 0$ [11].

FIG. 2: Dispersion relation of the pair excitations for $T = 0$. Thick lines: Second order. Thin lines: First order. Solid: $J = 0.029 \, U$. Dashed: $J = 0.025 \, U$.

see that one must suitably scale the hopping parameter [25, 26, 27]. When we define $\tilde{J} = 2DJ$, the contribution of the kth order chain diagram is proportional to $\tilde{J}^k$ because there exist $2D$ possibilities in a chain diagram for every hopping line to connect to neighboring sites. The lowest-order term neglected by that summation is the one-loop diagram in (8) which has two internal lines but only one free index and is, therefore, proportional to $2D J^2 = \tilde{J}^2/(2D)$. Thus, it vanishes in the limit of $D \to \infty$.

Taking now the one-loop diagram into account yields

$$\tilde{G}_1^{(2)}(\omega_m, \mathbf{k}) = \frac{1}{1/G_1^{(0)}(\omega_m) - J(\mathbf{k}) + \Sigma^{(2)}(\omega_m, \mathbf{k})} \, , \quad (10)$$

where $\Sigma^{(2)}(\omega_m, \mathbf{k}) = G_1^{(2B)}(\omega_m) / \left[G_1^{(0)}(\omega_m) \right]^2$ is the second-order self-energy with the value of the one-loop diagram $G_1^{(2B)}(\omega_m)$. The analytic formula for the phase boundary resulting from this formula is shown in Fig. 1. This result coincides in the limit of $T \to 0$ with the effective potential formalism employed in Ref. [9]. We emphasize that, unlike the first order (9), the one-loop corrected result depends on the system dimension in a non-trivial way. Furthermore, the corrections are larger in two than in three dimension which is consistent with the fact that the first-order results become exact in the limit $D \to \infty$. For finite temperature, the phase boundary is shifted towards larger values of J_c as thermal fluctuations suppress quantum correlations which are responsible for the formation of the superfluid. This effect, which occurs both in first and in second order, is most important between the Mott lobes as fluctuations are strongest when the average particle number is not near an integer value. The correction to the mean-field result arising from the one-loop diagram, visible in the difference between first and second order curve, plays an important role only near the tip of the Mott lobe. This feature stems from the fact that *quantum* fluctuation are notably increased when the system approaches the quantum critical point at the tip of the lobe [4]. Thus, we can say the quantum phase diagram consists of a thermally dominated region where the
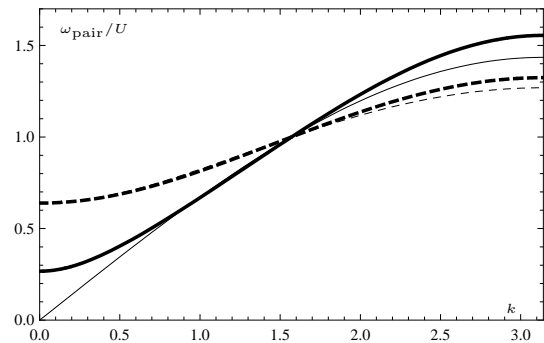
influence of thermal fluctuations is large and a quantum dominated region where the quantum corrections from the one-loop diagram are most important.

Excitation Spectrum: For a system in the Mott phase three different types of excitations exist. 1. The addition of a particle from the environment (particle excitation). 2. The removal of a particle (hole excitation). 3. The creation of a particle-hole pair (pair excitation). The last one is important from a physical point of view because it is also possible in an isolated system as realized in the current experiments. In the superfluid phase, there are additional excitations corresponding to fluctuations of the phase of the superfluid order parameter. However, these features can not be investigated within the present formalism but with the related effective action method [28].

In order to obtain the spectrum of the quasi-particles, which is given by the poles of the real-time Green function for finite temperature we must analytically continue our imaginary-time result. This is achieved by performing the replacement $i\omega_m \to \omega + i\eta$ with $\eta \to 0$ [17]. The first and second order, respectively, yield excitation spectra of which the former one agrees in the limit $T \to 0$ with the mean-field result from Ref. [7]. In the following we restrict ourselves to the most interesting case $D = 3$. Both finite temperature and one-loop corrections are most effective for small wave numbers, the former because the effect of temperature is the suppression of quantum correlations which mainly exist for long wavelengths, the latter because the dominant fluctuations near a quantum critical point are the ones with vanishing wave number as shown in Fig. 2

All spectra show a characteristic energy gap which vanishes at the critical point, i.e. at the value of J_c at the tip of a Mott lobe. Our prediction for the temperature dependence of this energy gap is shown in Fig. 3. As it is an experimentally accessible quantity [16] it could serve for determining the temperature of bosons in an optical lattice. Furthermore, we determine for both the quasi-particles and the quasi-holes an effective mass which is shown in Fig. 4. Note that they become massless at
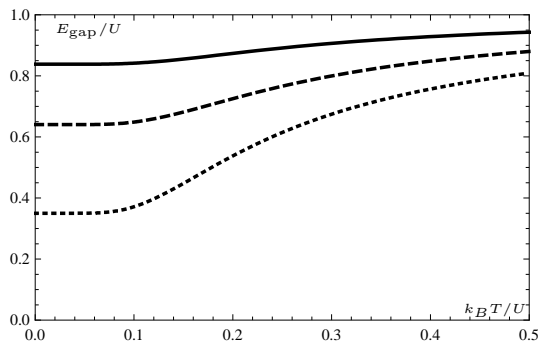
FIG. 3: Temperature dependence of gap for unit filling. Solid: $J = 0.008\,U$. Dashed: $J = 0.012\,U$. Dotted: $J = 0.025\,U$.
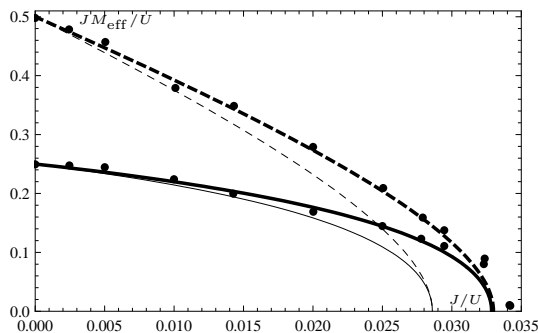

FIG. 4: Effective masses of quasi-particles (solid lines) and quasi-holes (dashed lines) for $T = 0$. Thick lines: Second order. Thin lines: First order. Dots: QMC data [11].

the critical point as a consequence of the U(1) symmetry breaking at the second-order phase transition.

Conclusion and Outlook: We have presented a powerful formalism to calculate the Green function for the Bose-Hubbard model in the Mott phase. It allowed us to improve the mean-field phase boundary in an analytic way for finite temperature. At absolute zero our result deviates from the recent Quantum Monte-Carlo studies of Ref. [11] by only 3% for $D = 3$. For finite temperature first analytic results beyond mean-field theory have been presented and the importance of both thermal and quantum fluctuations in the different regions of the phase diagram has been clarified. In addition, we have calculated the excitation spectrum of the quasi-particles and derived its effective masses and compared them to numerical findings. We have also investigated the characteristic energy gap and determined its temperature dependence. In order to obtain more accurate results, it would be desirable to extend the hopping expansion of the Green function to higher orders [29]. Furthermore, a promising way to obtain more insight into the superfluid phase would necessitate to combine the present technique with the effective action approach from Ref. [28].

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